

# Glutaric acid, cyclohexylmethyl 2-heptyl ester

**Inchi:** InChI=1S/C19H34O4/c1-3-4-6-10-16(2)23-19(21)14-9-13-18(20)22-15-17-11-7-5-8-12-17  
**InchiKey:** ADXZONHWOKTOJX-UHFFFAOYSA-N  
**Formula:** C19H34O4  
**SMILES:** CCCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1  
**Mol. weight [g/mol]:** 326.47

## Physical Properties

Property code	Value	Unit	Source
gf	-336.73	kJ/mol	Joback Method
hf	-876.05	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	76.24	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.792		Crippen Method
mvol	282.590	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	805.81	K	Joback Method
tc	1002.74	K	Joback Method
tf	440.59	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.26	J/molxK	805.81	Joback Method
cpg	988.46	J/molxK	969.92	Joback Method
cpg	974.49	J/molxK	937.10	Joback Method
cpg	959.30	J/molxK	904.28	Joback Method
cpg	942.89	J/molxK	871.45	Joback Method
cpg	925.21	J/molxK	838.63	Joback Method
cpg	1001.23	J/molxK	1002.74	Joback Method
dvisc	0.0000585	Paxs	805.81	Joback Method

dvisc	0.0000792	Paxs	744.94	Joback Method
dvisc	0.0001134	Paxs	684.07	Joback Method
dvisc	0.0001739	Paxs	623.20	Joback Method
dvisc	0.0002928	Paxs	562.33	Joback Method
dvisc	0.0005593	Paxs	501.46	Joback Method
dvisc	0.0012775	Paxs	440.59	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393586&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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